Normalization of scattering states and Levinson's theorem: reply to a comment by R. G. Newton [Helv. Phys. Acta 67, 20 (1994)]

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Abstract. Normalization of scattering states, Levinson's theorem and the high energy behavior of scattering phase shifts are discussed in the light of R. G. Newton's recent criticism.

1   Introduction

Recently R. G. Newton published a comment [1] criticizing the methods and the results of a paper published in this journal [2]. His criticism touches on a few key points of the subject and hence deserves a detailed reply. Here is the reply, point by point, to his criticism.

2   Normalization of scattering states

Let us first consider the case without a threshold resonance (i. e. either a finite solution with $k = 0$ does not exist or it is a bound state). We will return below to the (rather exceptional) case with a threshold resonance (sometimes called a half-bound state or a zero-energy solution). In this section we consider the case of a Schrödinger equation; the case of a Dirac equation is completely analogous and the relevant formulae can be found in [2].

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The usual statement on the normalization of scattering states for a central potential is

$$\int_0^\infty dr \, u_{kl}(r) \, u_{k'l}(r) = 2\pi \delta(k - k') \tag{2.1}$$

The question then arises of what happens in the limit $k \to k'$. Of course the right-hand side becomes infinite, but it is easy to see that the difference, between this equation and its free-particle counterpart, is finite. In [2] it was proven that

$$\int_0^\infty dr \, \left[u_{kl}^2(r) - v_{kl}^2(r) \right] = 2\eta_l'(k) \tag{2.2}$$

where $v_{kl}(r)$ are the free-particle wave functions and $\eta_l(k)$ is the phase shift.

Equations (2.1) and (2.2) can be put together as one compact equation

$$\int_0^\infty dr \, u_{kl}(r) \, u_{k'l}(r) = 2\pi \delta(k - k') + 2\eta_l'(k) \, \delta_{kk'} \tag{2.3}$$

where $\delta_{kk'} = 1$ if $k = k'$ and $\delta_{kk'} = 0$ otherwise.

Equation (2.3) is what R. G. Newton criticizes. As he put it: "He arrives at a modification of the usual quasi-orthogonality of the scattering wave functions in which the Dirac distribution is supplemented by a bounded function that differs from zero at only one point. In any context in which the Dirac distribution is meaningful, such a function is of course equal to zero, and its addition is of no consequence."

Admittedly, if the delta function on the right-hand side of (2.3) is interpreted strictly as a distribution, the addition of the second term is of no consequence and equations (2.3) and (2.1) are identical. However, the above criticism misses several points. One is that (2.3) is merely a short-hand description of the two equations (2.1) and (2.2), the validity of which is beyond any doubt. So that, if needed, any reference to (2.3) can be avoided.

A deeper point is that the Dirac delta function and a distribution are not exactly identical concepts, e. g. the delta function on the right-hand side of (2.1) or (2.3) cannot be interpreted as a distribution in the usual mathematical sense. The proof of this statement is as follows. Assume that this delta function is a distribution. However, for the left-hand side of (2.1) it perfectly makes sense to subtract its free-particle counterpart and then put $k = k'$. The result is finite and given in (2.2). On the other hand, for the right-hand side of (2.1) such an operation does not make sense (or its outcome is ambiguous), if the delta function is interpreted as a distribution. Hence the left- and the right-hand side of (2.1) cannot be the same object and the conclusion is: the right-hand side of equation (2.3) is a modification of the usual notion of a distribution.

The mathematical notion of a distribution is based on a class of all possible limiting processes, whereas in quantum theory the Dirac delta function is always either a particular limiting process or a particular class of limiting processes with a fixed physical interpretation of the parameters involved.[2] Having this in mind there is no danger of ambiguities for the use of equation (2.3).

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[2]For instance, in the usual calculation of a differential cross section in quantum field theory one has to square a Dirac delta function, which is done unambiguously using a particular physically motivated limiting process. From the point of view of a distribution this does not make sense.

3 Levinson's theorem

Consider the completeness relation

$$\sum_{\epsilon_l \leq 0} u_{\epsilon_l l}\left(r\right) u_{\epsilon_l l}\left(r'\right) + \int_0^\infty \frac{\mathrm{d}k}{2\pi} u_{kl}\left(r\right) u_{kl}\left(r'\right) = \delta\left(r - r'\right) \tag{3.1}$$

where the sum runs over the bound and the integral over the scattering states.

If the right-hand side of (3.1) is interpreted as a Dirac delta function (i. e. as a class of limiting processes which are independent of the potential) and not as a usual distribution, we can subtract from (3.1) its free particle counterpart and put $r = r'$. The delta functions cancel and we obtain

$$\sum_{\epsilon_l \leq 0} u_{\epsilon_l l}^2\left(r\right) + \int_0^\infty \frac{\mathrm{d}k}{2\pi} \left[u_{kl}^2\left(r\right) - v_{kl}^2\left(r\right)\right] = 0 \tag{3.2}$$

Integrating (3.2) over r and substituting (2.2), we obtain the Levinson theorem

$$\eta_l\left(0\right) = n_l \pi \tag{3.3}$$

for the case of a Schrödinger equation, where n_l is the number of bound states. If the same is carried out for the case of a Dirac equation (see ref. [2] for the details), the result is

$$\eta_{m\kappa}\left(0\right) + \eta_{-m,\kappa}\left(0\right) = \left(N_\kappa^+ + N_\kappa^-\right)\pi \tag{3.4}$$

where N_κ^+ is the number of positive and N_κ^- is the number of negative energy bound states.[3]

Looking at (3.4) it is natural to ask whether a stronger statement of Levinson's theorem is possible, valid for the positive and negative energy phase shifts separately. It turns out to be the case [3]. The clue to derive such a stronger statement of Levinson's theorem is simple: consider the second order (iterated) Dirac equation and take the limit $k \to 0$. In this nonrelativistic limit[4] the second order Dirac equation becomes identical to a Schrödinger equation, so that at $k = 0$ one can relate the phase shifts of a Dirac equation to the phase shifts of a corresponding Schrödinger equation. The stronger statement of Levinson's theorem obtained in this way is:

$$\eta_{m\kappa}\left(0\right) = n_\kappa^+ \pi \tag{3.5}$$

$$\eta_{-m\kappa}\left(0\right) = n_\kappa^- \pi \tag{3.6}$$

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[3]More precisely we obtain

$$\eta_l\left(0\right) = \eta_l\left(\infty\right) + n_l \pi$$

for the case of a Schrödinger equation, and

$$\eta_{m\kappa}\left(0\right) + \eta_{-m,\kappa}\left(0\right) = \eta_{\infty\kappa}\left(\infty\right) + \eta_{-\infty,\kappa}\left(\infty\right) + \left(N_\kappa^+ + N_\kappa^-\right)\pi$$

for the case of a Dirac equation. However, we are free to put $\eta_l\left(\infty\right) = 0$ and $\eta_{\infty\kappa}\left(\infty\right) + \eta_{-\infty,\kappa}\left(\infty\right) = 0$.

[4]It is an interesting fact that such a non-relativistic limit which, from the physical point of view, is a most natural one, does not coincide with the usual expansion based on the Foldy-Wouthuysen scheme (see [4]).

where n_κ^+ is the number of positive and n_κ^- the number of negative energy nodes of the $k = 0$ solution of the Dirac equation. Unlike the case of a Schrödinger equation, there is a subtlety here: for a given energy sign the number of bound states may not equal the number of nodes of a $k = 0$ solution, i. e. in general $N_\kappa^+ \neq n_\kappa^+$ and $N_\kappa^- \neq n_\kappa^-$. The equality holds only for the total numbers:

$$N_\kappa^+ + N_\kappa^- = n_\kappa^+ + n_\kappa^- \tag{3.7}$$

The generality and simplicity of the above proof of Levinson's theorem speaks for itself, and can be viewed as a confirmation of the validity and usefulness of the above discussion on the normalization of scattering states. Notice that we did not have to assume anything explicit about the potential. The only implicit assumption is that the potential decays faster than $1/r^2$ at large distances, which is sufficient for the validity of (2.2).

However, when in ref. [2] this proof was extended to the case with a threshold resonance, a surprising result was obtained:

$$\eta_l(0) = (n_l + q)\pi \tag{3.8}$$

in the case of a Schrödinger equation, and

$$\eta_{\pm m\kappa}(0) = \left(n_\kappa^\pm + q\right)\pi \tag{3.9}$$

in the case of a Dirac equation, where either $q = 0$, or $q = \frac{1}{4}$, or $q = \frac{1}{2}$. For the case with a threshold resonance $q = 0$ can be ruled out and $q = \frac{1}{2}$ is what one would have expected. The surprise is in the possibility of allowing for $q = \frac{1}{4}$, which is the subject of R. G. Newton's criticism. From the point of view of a conventional proof of Levinson's theorem, where there is always a certain restriction on the potential, the case $q = \frac{1}{4}$ cannot be ruled out completely. However while the paper [2] was in press it was found that the derivation of the normalization integral actually implies a certain constraint which was overlooked in [2] and which rules out the case $q = \frac{1}{4}$. This is the reason why in a subsequent paper [3] the case $q = \frac{1}{4}$ was not mentioned. Meanwhile M. Sassoli de Bianchi [5] investigated the problem within the framework of one spatial dimension and came to the same conclusion. In the following section these matters are considered in more detail.

4   The case with a threshold resonance

Assume that the coupling constant is tuned such that a finite, $k = 0$ solution (threshold resonance) exists. By examining its asymptotic behavior at large distances, it is easily seen that such a solution is normalizable (i.e. a bound state), unless $l = 0$, in the case of a Schrödinger equation, and $\kappa = -1$, $\epsilon = m$ or $\kappa = 1$, $\epsilon = -m$, in the case of a Dirac equation.[5] Hence in this section $l = 0$, in the case of a Schrödinger equation, and $\kappa = \pm 1$, in the case of a Dirac equation.

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[5]Notice that, for a given angular momentum, at most one threshold resonance is possible, either with $\epsilon = m$ or with $\epsilon = -m$.

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According to [2] in the presence of a threshold resonance (2.2) becomes modified according to

$$\int_0^\infty dr \, \left[u_{k0}^2 (r) - v_{k0}^2 (r) \right] = 2\eta_0' (k) + 2\pi\delta (k) \sin^2 \eta_0 (k) \tag{4.1}$$

As in section 3, integrating (3.2) over r and substituting (4.1), we obtain Levinson's theorem for the case with a threshold resonance

$$\eta_0 (0) = n_0\pi + \frac{\pi}{2} \sin^2 \eta_0 (0) \tag{4.2}$$

Equations (4.1) and (4.2) are valid for a Schrödinger equation. In the case of a Dirac equation, as was mentioned in the preceding section, one can rewrite the Dirac equation at $k = 0$ as an ordinary Schrödinger equation and use (4.2) to obtain the stronger statement of Levinson's theorem for a Dirac equation:

$$\eta_{\pm m\kappa} (0) = n_\kappa^\pm \pi + \frac{\pi}{2} \sin^2 \eta_{\pm m\kappa} (0) \tag{4.3}$$

where n_κ^+ is the number of positive and n_κ^- the number of negative energy nodes of the $k = 0$ solution.

Equation (4.2) was first derived in ref. [6]. The authors did not check for all solutions of this equation but instead were content by verifying that (3.8) for $q = 0$ and $q = \frac{1}{2}$ is a solution of (4.2). Equations (4.2) and (4.3) were derived independently in ref. [2] and it was pointed out that there is a third solution with $q = \frac{1}{4}$. However it was not noticed that the derivation of (4.1) also implies

$$\sin [2\eta_l (0)] = 0 \tag{4.4}$$

This constraint rules out the case $q = \frac{1}{4}$ in (3.8).[6]

To understand how this constraint comes about, we now consider the derivation of (4.1) in more detail (section 2.1 of ref. [2]). We start with the exact identity

$$\int_0^R dr \, u_{kl}^2 (r) = \frac{1}{2k} \left[u_{kl}' (R) \, \partial_k u_{kl} (R) - u_{kl} (R) \, \partial_k u_{kl}' (R) \right] \tag{4.5}$$

and assume that the potential $V (r)$ vanishes for $r \geq R$. Then the right-hand side of (4.5) depends only on the asymptotic wave functions and thus can be calculated. The result is

$$\int_0^R dr \, u_{kl}^2 (r) = 2R + 2\eta_l' (k) - (-1)^l \frac{1}{k} \sin [2kR + 2\eta_l (k)] \tag{4.6}$$

Subtracting from (4.6) its free-particle counterpart and expanding the sinus, we obtain

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[6]The situation for a Dirac equation is completely analogous and the constraint is

$$\sin [2\eta_{\pm m\kappa} (0)] = 0$$

This constraint rules out the case $q = \frac{1}{4}$ in (3.9).

$$\int_0^R dr \left[u_{kl}^2(r) - v_{kl}^2(r) \right] = 2\eta_l'(k) + (-1)^l \left\{ 2 \sin^2 \eta_l(k) \frac{\sin(2kR)}{k} - \frac{\sin[2\eta_l(k)]}{k} \cos(2kR) \right\}$$
(4.7)

The second term in curly parenthesis possesses a k^{-1} singularity unless $\sin[2\eta_l(0)] = 0$. In the case with a threshold resonance, where the $k = 0$ state is part of scattering states, such a singularity is intolerable (for instance, the integral over k in (3.2) includes the point $k = 0$ in this case). Hence the constraint (4.4) must be satisfied. The derivation of (4.1) is complete now, if one sends $R \to \infty$.

5 High energy limit

In [2] it was shown that the high energy behavior of the scattering phase shifts is

$$\eta_l(k) \xrightarrow[k\to\infty]{} k \int_0^\infty dr \left[\sqrt{1 - \frac{2m}{k^2} V(r)} - 1 \right],$$
(5.1)

in the case of a Schrödinger equation, and

$$\eta_{\epsilon\kappa}(k) \xrightarrow[k\to\infty]{} k \int_0^\infty dr \left[\sqrt{1 - \frac{2\epsilon}{k^2} V(r)} - 1 \right],$$
(5.2)

in the case of a Dirac equation. Obviously, if the potential V is less singular than $1/r$ at the origin, then (5.1) and (5.2) lead to the well known results

$$\eta_l(\infty) = 0$$
(5.3)

in the case of a Schrödinger equation, and

$$\eta_{\epsilon\kappa}(k) \xrightarrow[k\to\infty]{} = -\frac{\epsilon}{|\epsilon|} \int_0^\infty dr \, V(r)$$
(5.4)

in the case of a Dirac equation.

R. G. Newton doubts the validity of (5.1) and (5.2): "His change of variables leads, without comment, to a highly singular equation on a complex contour, and it is not clear whether his manipulations are valid."

This criticism is without foundation, since the equations, which were used to derive (5.1) and (5.2), become singular only at certain finite values of k. Taking into account the fact that these equations are local in k, such singular behavior is irrelevant to the high energy limit $k \to \infty$.

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